Chemical Communications

Notice to Authors, 1980

Refereeing Policy—Chemical Communications is intended as a forum for preliminary accounts of original and significant work that is likely to prove of wide general appeal or of exceptional specialist interest, and its scientific content will be restricted to such communications. The policy of the Society remains that only a fraction of research work warrants duplicate publication, and communications will be subject to scrutiny by referees. Urgent need for the broadcast of the information must outweigh the general desire to avoid multiple publication. Priority is therefore not an important factor. The needs of the potential user must be considered, not the needs of the authors.

Authors are therefore required to submit, together with three copies of the communication, two copies of a statement of the reasons why urgent publication is desirable. Further, authors are encouraged to indicate, early in the manuscript, the urgent or novel aspect of the work for the benefit of readers.

It should be noted that communications are normally restricted to *ca.* 600 words (1 printed page, to include formulae, Tables, and Figures); supplementary data not to be published may, however, be submitted for the referees' consideration.

Acceptance by two independent referees will lead to immediate publication; communications will not be rejected on the recommendation of one referee only, and authors of refused communications will have the right to appeal, through the Editor, to the Journals Committee.

Short articles which have the detail of content and argument appropriate to the definitive paper but lack urgency should be submitted to the Journal.

Administration—An acknowledgement of receipt will be sent by return of post to the author submitting a manuscript. If, within a reasonable time such a document has not been received, the author is advised to contact the Editor. As soon as the referees' recommendations have been received by the Editor, authors will be informed whether the communication has been accepted.

Urgency—The Journals Committee has instructed the editorial staff of *Chemical Communications* that if authors fail to reply to referees' recommendations, or to return proofs, within one month of the date of dispatch the communication concerned may be regarded as abandoned.

Editing—Editing will be as light as is consistent with a reasonable standard of presentation, clarity of expression, and the conciseness required in *Chemical Communications*.

Manuscripts—Careful attention to the following points will aid rapid publication.

(*a*) Three copies of the manuscript *must* be provided. One should be a top-quality original, in double-line spacing, typed on one side of the sheet only. Good quality non-greasy paper must be used. Margins of at least 1½ inches must be left at the top, bottom, and left-hand side.

(*b*) The first page should be set out as follows:

(i) Title of communication, capitals for first letter of each noun and adjective *only*.

Note: The inclusion of "Series or Part numbers" in the title of communications is not allowed.

(ii) Authors' names, with one forename for each author, (doubly underlined) preceded by "By" on the same line.

The name of the author who will deal with correspondence arising out of publication of the communication will be indicated by an asterisk (*) placed after it.

(iii) Authors' address, singly underlined and enclosed in parentheses.

(iv) An extra line of space.

(v) A one-sentence summary.

(vi) An extra line of space.

(vii) Main text, first paragraph not indented, with the first word doubly underlined.

(*c*) Spacings must be those required in print, *e.g.*, each paragraph must be indented. A space must be left after numerals (except where these occur in chemical names), when these qualify units (*e.g.*, 3 g), but not when they are multiples (10^3k).

(*d*) Attention should be paid to underlining, and punctuation (or its absence) in symbols and chemical names. Greek letters should be explained by marginal notes (*e.g.*, Gk nu) and *not* underlined.

(*e*) Alterations must be made by complete erasure, or by crossing out the error and writing the correct version above it.

(*f*) Bibliographic references are indicated in the text by superior numerals and must be *cited* in numerical sequence. The corresponding footnotes should include the author's initials given before the surname and should be set out on a separate sheet.

(*g*) Captions to illustrations should preferably be presented on a separate sheet.

(*h*) Displayed formulae should be carefully and unambiguously drawn on a separate sheet. They should be numbered for ease of reference in the text.

(i) Illustrations should be good-quality Indian ink drawings suitable for immediate reduction to about 2 inches in width Lettering should be clearly but lightly inserted in pencil—the printer will set it in type Drawings requiring additional draughtsmanship are likely to cause delay

The Title—The choice of the wording of the title is of greatest importance, since it is from this that the important keywords used in information retrieval are taken The title should clearly and accurately indicate the contents of the communication and should be expressed in adequate scientific terms that can function as 'points of entry' for retrieval purposes Brevity in a title, though desirable, should be balanced against its accuracy and usefulness

The Summary—The *Summary* should be a one-sentence account of the discovery being announced It must clearly indicate the content which makes the communication important or urgent and be informative rather than indicative, *i e* be of the form

"Reaction of sodium with ethanol in dry benzene gives the monomeric sodium ethoxide" and not "The reaction of sodium with ethanol in dry benzene has been studied"

Nomenclature—For many years the Society has actively encouraged the use of standard I U P A C nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers Although the I U P A C rules for naming organic compounds have now gained wide acceptance amongst chemists, mainly because they have been in existence for a number of years, those for naming inorganic compounds are of more recent origin and for this reason their acceptance is less general

In order to encourage authors to use I U P A C nomenclature rules when drafting papers, attention is drawn to the following publications in which both the rules themselves and guidance on their use are given

'Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H,' 1979 edition, Pergamon, Oxford, 1979

'Nomenclature of Inorganic Chemistry,' 2nd edition, Butterworths, London, 1971

'Manual of Symbols and Terminology for Physicochemical Quantities and Units,' 1979 edition, Pergamon, Oxford, 1979

In addition to the above publications, provisional rules for the naming of organometallic compounds, amino-acids, carbohydrates, carotenoids, and steroids, and rules of stereochemistry are available from the

I U P A C Secretariat,
Bank Court Chambers,
2—3 Pound Way,
Cowley Centre,
OXFORD OX4 3YF

It is recommended that where there are no I U P A C rules for the naming of particular compounds or authors find difficulty in applying the existing rules, they should seek the advice of the Society's editorial staff

Brevity—In order that the maximum number of communications can be published in the space available, individual articles must be as brief as possible (see para 3 of Notice), and should be restricted to the central urgent theme, historical introduction, experimental detail, physical data, and mechanistic conjecture will normally not be published, and detail essential to the proof of soundness should be given in a covering letter for assessment by the referees

Illustrations, tables, and graphic formulae are space-consuming and will be published only if vital to the exposition of the central theme

Acknowledgements—Only personal acknowledgements and those indicating financial support of the research will be published

Footnote Indications—Because of their special use to indicate the author to whom correspondence should be addressed, asterisks are not available to indicate footnotes to the main text

They may, of course, continue to be used in recognised specialised scientific terms (*e g* , $n \rightarrow \pi^*$ transitions)

Proofs—Proofs will normally be sent by first-class mail—by airmail where appropriate—to the person submitting the article or to the person designated by him

Reprints—A reprint order form will be circulated to authors with proofs Its early return will facilitate production both of *Chemical Communications* and of the reprints

The reprint will have a self-cover, *i e* , be printed as a four-page leaflet with the title and reference repeated on the front page

Chemical Communications

Notice to Authors

Supplementary Crystallographic Data

(i) *General*

Following its inception at the end of 1976, the scheme for the deposition† with the Cambridge Crystallographic Data Centre (C C D C) of supplementary information for articles published in *Chemical Communications* reporting the crystallographic determination of the structures of compounds containing organic carbon has in general operated quite satisfactorily The surprisingly large number of requests the C C D C has received for deposited information seems to indicate that the scheme is providing a useful and necessary service

However, the C C D C has experienced difficulties in dealing with some of the supplementary material supplied and authors are strongly urged to note the points in section (ii) below to aid the C C D C staff in processing the supplementary material and making it available to interested readers The overall situation with regard to supplementary crystallographic material is also somewhat anomalous in that only molecules containing organic carbon are included in the C C D C scheme, this anomaly will be removed in future as a result of the establishment of an inorganic structural database at the University of Bonn, West Germany [see section (iii)]

(ii) *Compounds containing Organic Carbon*‡

The problems the C C D C have experienced have arisen for two main reasons —

(*a*) In many cases authors have supplied computer listings which contain redundant information, and these listings require extensive editing before the data can be keyboarded The C C D C requires *only* a table of atomic co-ordinates and a table of intramolecular distances between bonded atoms Intermolecular distances, and intramolecular distances between non bonded atoms, are *not* required

Computer programs are available that produce well organized tabulated listings of atomic co-ordinates and bond lengths separate from other information, if such a program has not been used, authors are strongly urged to provide a retyped version § of the required data Additional information (*e g* bond angles) may be of assistance to the C C D C if any problems arise during their internal consistency check on the deposited data, but it must be emphasized that the C C D C 's prime concern is with *atomic co-ordinates* and *bond lengths* only

In some communications, the structural diagram may contain a fairly extensive listing of bond lengths, however, in such cases it would assist the C C D C staff greatly if authors would also provide a separate table including all bond lengths

(*b*) Some of the printout that has been provided in the past has been produced on line-printers with poor quality ribbons resulting in a very low contrast between print and paper This has led to serious problems in fulfilling readers' requests for atomic co-ordinates Authors are therefore requested either to ensure that their computer output is of suitable quality for it to be photocopied, or, if their output is relatively faint and indistinct, to provide a retyped version of the tabulated atomic co-ordinates and bond lengths

On a general point, readers should note that, although data can be obtained, on request, at any time, the C C D C work schedule requires approximately 3 months for the checking of the data

(iii) *Compounds not containing Organic Carbon*

The C C D C database is restricted to compounds containing organic carbon ‡ and so it has not been possible so far to include inorganic compounds in the deposition scheme However, an inorganic structural database has been established at the University of Bonn, and it will now be possible for data for inorganic compounds to be deposited and for the atomic co ordinates to be made available to interested readers The full address for the inorganic database is

Institut fur Anorganische Chemie,
Universitat,
Gerhard-Domagk-Str 1,
D–5300 Bonn 1,
WEST GERMANY,

and correspondence should be addressed to Prof Dr G Bergerhoff

In general, the same considerations as are outlined in the Notices to Authors regarding the C C D C scheme and in sections (ii), (*a*) and (*b*), above will apply, with the important addition that the organisers of the Bonn database wish to process *all* contact distances, and, in addition, vibrational parameters For inorganic structures, therefore, authors are requested to provide good quality print-out, or retyped versions, of *atomic co-ordinates*,

† See Notice to Authors, *J C S Chem Comm* , 1977, p 3 1978, p 3

‡ These include co ordination compounds containing organic ligands or counter ions, but exclude, for example, metal carbonyls or cyano complexes in the absence of other organic components A convenient definition has been the following — The compound contains carbon but compounds where the carbon is present only as *e g* CO_3^{2-}, CN, CNS, CO, *etc* are excluded

§ The original Notices to Authors requested print out for all supplementary material to avoid the possibility of transcription errors introduced during retyping In view of difficulties in processing unsuitable print out, however, the C C D C would now much prefer to receive retyped data if the original computer print out is unsuitable

interatomic distances, and *vibrational parameters* (in the form of U_{ij} with units of Å^2 or specified by a given formula). When a communication is published, this material will be sent by the Society initially to the C.C.D.C., who will then forward it to the University of Bonn. Copies of the atomic co-ordinates will be available, on request, from the University of Bonn. If authors are uncertain as to whether the molecule whose structure they are reporting would be considered to contain organic carbon, they should include the vibrational parameters in the supplementary material so that they are available for inclusion in the inorganic database if necessary. As is the case for data currently included in the C.C.D.C. database, supplementary material for inorganic compounds should be submitted with the manuscript initially so that it may be considered by the referees.

(iv) *Structure Factor Tables*

Structure factor tables are not deposited in the C.C.D.C. database, and will not be deposited at the University of Bonn either. However, if an author is not intending to include details of a structure determination as part of a full paper in the future, the structure factor table should be sent with the communication as supplementary material for deposition with the British Library, Lending Division. This applies to 'organic' and 'inorganic' compounds alike.

(v) *Summary*

Supplementary data will be deposited with the C.C.D.C. for crystal structures of 'organic' compounds, and with the University of Bonn for 'inorganic' compounds. Supplementary data should include the following.

(*a*) Unit cell data [*i.e.* unit cell parameters with standard deviations, space group, number (Z) of formula units per cell] if not listed in the manuscript. A definition of the formula unit must be given {*e.g.*

$$Z\ [Ca_{2\cdot71}\ Mg_{0\cdot29}\ (PO_4)_2] = 21\}.$$

(*b*) Atomic co-ordinates with corresponding interatomic distances (for 'organic' compounds, only intramolecular distances between bonded atoms are required).

(*c*) Vibrational parameters (in the form of U_{ij} with units of Å^2 or specified by a given formula) for 'inorganic' substances only.

The lists in (*b*) and (*c*) should take the form of *either* readable (and reproducible) tabulated computer lists *or* typed lists.

Structure factor tables are only required if it appears that the *Chemical Communications* article will be the only report of a particular piece of work. If this is the case, authors should make this clear when submitting their manuscript.